

5-Ethyl-1-methyl-5-(1-phenylethyl)pyrimidine-2,4,6(1H,3H,5H)-trione  
61346-87-0 | DTXSID60818264

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 148 °C

Global applicability domain: Inside

Local applicability domain index: 4.37e-01

Confidence level: 3.24e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Mephobarbital</div> <div>Measured: 176</div> <div>Predicted: 155</div>	<div>Image not found</div> <div>Bucolome</div> <div>Measured: 84.0</div> <div>Predicted: 107</div>	<div>Image not found</div> <div>Lenacil</div> <div>Measured: 316</div> <div>Predicted: 272</div>
<div>Image not found</div> <div>Metharbital</div> <div>Measured: 151</div> <div>Predicted: 132</div>		